New Monotone Finite Volume Scheme for Anisotropic Diffusion

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Predictive numerical simulations of subsurface processes require not only more sophisticated physical models but also more accurate and reliable discretization methods for these models. We have studied a new monotone finite volume scheme for diffusion problems with a heterogeneous anisotropic material tensor [1]. Examples of anisotropic diffusion include diffusion in geological formations, head conduction in structured materials and crystals, image processing, biological systems, and plasma physics. Development of a new discretization scheme should be based on the requirements motivated by both practical implementation and physical background. This scheme must meet the following conditions:

- -be locally conservative;
- -be monotone, i.e., preserve positivity of the differential solution;
- -be applicable to unstructured, anisotropic, and severely distorted meshes;
- -allow arbitrary diffusion tensors;
- -result in sparse systems with a minimal number of non-zero entries;
- -have higher than the first-order accuracy for smooth solutions.

The discretization methods used in existing simulations, such as the mixed finite element (MFE) method (Fig. 1), finite volume (FV) method, mimetic finite difference (MFD) method, and multipoint flux approximation (MPFA) method, satisfy most of these requirements except the monotonicity. They fail to preserve positivity of a continuum solution when the diffusion tensor is heterogeneous and anisotropic or the computational mesh is strongly perturbed. For instance, in simulations of a subsurface transport, a negative discrete solution of the pressure equation implies nonphysical Darcy velocities and hence wrong prediction of a contaminant transport.

Recently a few nonlinear monotone schemes have been suggested [2,3]. We studied schemes based on the nonlinear flux formula proposed in [3]. We rectified the LePotier's scheme for the case of unstructured triangulations and full diffusion tensors by giving correct positions of reference points. To improve robustness of the scheme, we proposed an alternative interpolation technique [4]. We gave the first proof of scheme monotonicity for the steady diffusion equation. We studied numerically important features of the scheme such as violation of the discrete maximum principle and impact of the diffusion anisotropy on the scheme convergence. We extended the scheme to shape regular polygonal meshes and heterogeneous isotropic diffusion tensors.

The mixed form of the diffusion equation includes the mass conservation equation and the constitutive equation:

$$\mathrm{div}\mathbf{q} = Q,$$
$$\underline{\mathbf{q}} = -\mathbb{D}\,\mathrm{grad}C,$$

where $\mathbb{D}$ is the diffusion tensor, Q is the source term, and $\mathbf{q}$ is the flux of concentration C.

All the methods mentioned above use the same discretization of the mass conservation equation and differ by their approximation of the flux (constitutive) equation. In the nonlinear finite volume scheme a *reference* point is defined for each mesh cell T to approximate the concentration C. The position of the reference point depends on the geometry of T and value of the diffusion tensor. For isotropic diffusion tensors and triangular cell T, the center of the inscribed circle is the acceptable position for the reference point.

The flux $\mathbf{q}$ is approximated at the middle of each mesh edge using a weighted difference of concentrations in two neighboring cells. Nonlinearity comes from the fact that these weights depend on a concentration at the edge vertices. To approximate solution at a mesh vertex, a linear interpolation method has been proposed in [3]. This method uses the three closest reference points, which form a triangle containing the vertex. We found out that this method is not robust for problems with strong anisotropy and sharp gradients. We proposed the *inverse distance weighting* interpolation method [4] for such a problem type. This method uses values at all reference points from the closest neighborhood of the vertex. Numerical experiments show that the new method is more stable for highly anisotropic problems.

The nonlinear finite volume method results in a sparse system whose dimension is equal to the number of mesh cells T. For triangular meshes, the matrix of this system has at most four nonzero elements in each row. To solve the nonlinear algebraic problem we use the Picard iterative method, which guarantees monotonicity of the discrete solution for all iterative steps.

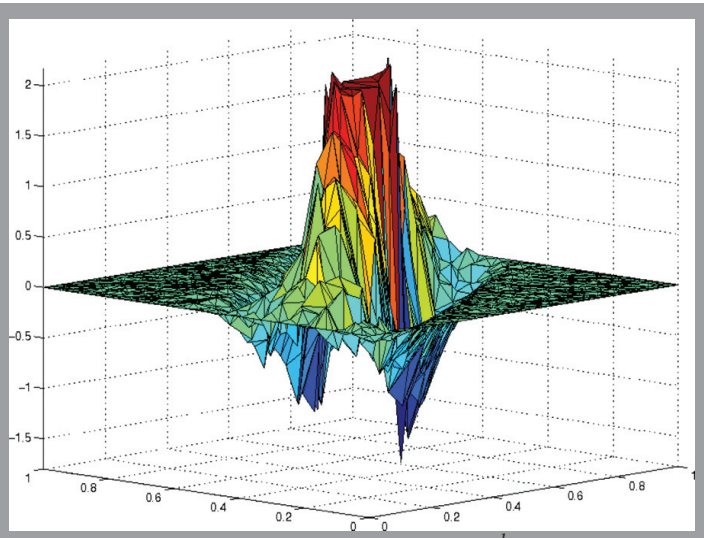

Fig. 1. Mixed finite element method, $C^h_{min} = -1.7$

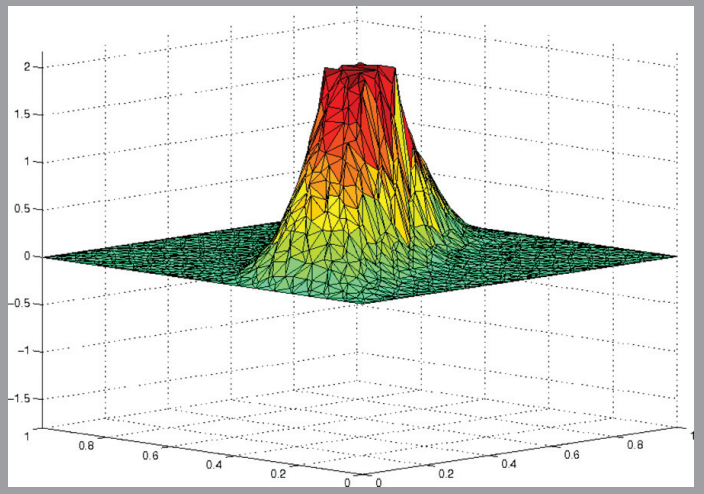

Fig. 2. Nonlinear finite volume method, $C^h_{min} = 0$

Profile of solution $C^h(x,y)$ on the distorted triangular grid. Domain: unit square with the hole in the center. Problem: diffusion equation with highly anisotropic tensor. Ratio of tensor's eigen-values is 10^3. Tensor is rotated with respect to coordinate axes on 60° clockwise. $C^h = 2$ on the hole, $C^h = 0$ on the boundary of unit square. Analytical solution satisfies maximum principle, $0 \le C(x,y) \le 2$. The MFE method produces nonphysical solution with strong negative values.

The computational results demonstrate the flexibility and accuracy of the scheme [2]. For sufficiently smooth solutions, we achieve the second-order convergence for concentration C and at least the first-order for flux **q** in a mesh-dependent L_2-norm. For nonsmooth, highly anisotropic solutions we observe at least the first-order convergence for both unknowns.

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